generated trajectories, various estimators can be accurately evaluated such as the propagator, the first time of passage, the mean square displacement etc. Furthermore, these estimators can be ensemble averaged which is much more selective than time average estimators. We applied this method to the GlyR receptor diffusion dynamics in the neuronal plasma-membrane.

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4081-Pos Board B809

High Density Single Particle Tracking with Various Probes

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Single Particle Tracking (SPT) is a set of single molecule techniques that identify and characterize the motion of individual particles in a medium. High Density Single Particle Tracking (HDSPT) is a subset of advanced SPT techniques designed to overcome some of the limitations of current SPT methods, primarily to compensate for poor statistical information due to low trajectory counts per observed area as seen in conventional SPT. Quantum Dots (QDs), Fluorogen Activating Peptides (FAPs), and Organic Dyes are recognized probes that have been used in SPT experiments. QDs are very bright, photo stable probes with blinking dictated by power law behaviors. A FAP will bind to a receptor and activate, emitting photons at a constant rate and intensity until it bleaches. ODs have emission behaviors characterized by Jablonski diagrams; depending on the particular OD and buffer combination, they may blink or bleach. Variable emission dynamics provide a challenge in SPT analysis because it requires localization techniques that can properly account for varying probe behaviors. We have modified our multi-emitter fitting algorithm [1] with a Bayesian approach in order to localize overlapping probes with variable intensity profiles. This advancement in localization capturing allows us to overcome one of the more difficult challenges present in high density SPT- reliable probe identification in high density regions. We have tested our modified SPT software on simulated data as well as on live Rat Basophil Leukemia (RBL) cells with various probes to demonstrate our approach to high density SPT.

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4082-Pos Board B810

Cell Adhesion Sensitivity to Cell Size and Surface Receptor Densities

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Using a Monte Carlo based code in conjunction with a Weighted Histogram Analysis Method (WHAM) we explore the impact of the size of Cells/Nanocarriers on their binding to functionalized surfaces. In our study we vary the size of Cells/Nanocarriers between 50 nm up-to 1 micron and also vary the number of receptors on these Cells/Nanocarriers such that the surface coverage of receptors ranges between 45%-95%. We adopt a two level framework: (i) where we explicitly model all surface receptors and their interactions with the surfaces for the smaller Cell/Nanocarrier systems (< = 200 nm) and (ii) for larger Cells/Nanocarriers we perform coarse grained simulations where we develop receptor ligand interaction potentials for smaller regions of the Cells and incorporate them to then derive a potential of mean force (PMF) for the full Cell surface interactions. We compare the results from the two approaches to establish the validity of the coarse graining methodology. We then evaluate the sensitivity of predicted equilibrium dissociation constants to cell size and surface coverage by receptors.

4083-Pos Board B811

Game on, Science - How Video Game Technology may Help Biophysicists Tackle Visualization Challenges

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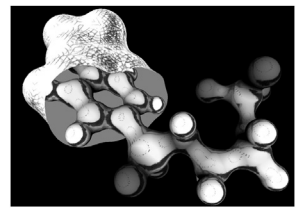
The video games industry develops ever more advanced technologies to improve rendering, image quality, ergonomics and user experience of their creations providing very simple to use tools to design new games. In biophysics, only a small number of experts with specialized know-how are able to design interactive visualization applications, typically static computer programs that cannot easily be modified. Are there lessons to be learned from video games? Could their technology help us explore new molecular graphics ideas and render graphics developments accessible to non-specialists?

This approach points to an extension of open computer programs, not only providing access to the source code, but also delivering an easily modifiable and extensible scientific research tool. In this work, we use the Unity3D game engine to develop a visualization application for research and education. Classical and novel representations such as molecular structures, HyperBalls, surfaces, animated chemical reactions, animated electrostatic field lines and biological networks can be decorated with powerful, artistic and illustrative rendering methods. Our prototype is easily modifiable and extensible and may serve others as starting point and platform for their developments.



4084-Pos Board B812

Loos: A Tool for Making New Tools for Analyzing Molecular Simulations

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We have developed LOOS (Lightweight Object Oriented Structure-analysis) as a tool for making new tools for analyzing molecular simulations. LOOS is an object-oriented library written in C++ with a Python interface and was designed to facilitate the rapid development of new methods for structural analysis in either C++ or Python. In addition, LOOS includes over 130 pre-built tools for common structural analysis tasks including 3D histograms for visualization, hydrogen bonding patterns, and assessing simulation convergence. LOOS also includes a set of libraries and tools for performing elastic network model calculations. LOOS supports reading the native file formats of most common simulation packages, such as Amber (including NetCDF-formatted), CHARMM, Gromacs, NAMD, and Tinker. LOOS can also write NAMD formatted PDB and DCD files. A dynamic atom selection language, based on the C expression syntax, is included in the library and is easily accessible to the tool writer. Through modern C++ design, LOOS is both simple to use, requiring knowledge of only 4 core classes, and easy to extend. LOOS makes extensive use of Boost and the Standard Template Library for correctness and ease of use, and relies on ATLAS for high performance numerical routines.

4085-Pos Board B813

CHARMM-Gui Pace Cg Builder for Solution, Micelle, Bilayer and Vesicle Simulations

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Coarse-grained and multi-scale simulations are widely used to study large biological systems nowadays. However, building the simulation system is not trivial in some occasions. We have developed the CHARMM-GUI PACE CG simulator for building solution, micelle, bilayer and vesicle systems using the PACE force field, a united-atom model for proteins, and Martini, a coarse-grained force field for water, ion and lipids. The qualities of the output systems are validated by simulation of various examples and comparison of the coarse-grained simulation to all-atom simulation. We expect this module to be a useful tool for modeling large, complicated systems.

4086-Pos Board B814

Calculator for Mutual Information Between a Discrete and a Continuous Data Set

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Mutual information (MI) is in many ways an ideal statistic for detecting relationships between two data sets. MI is easy to calculate when both data sets are discrete, but not when one or both data sets are real-valued. An accurate method for calculating MI between two real-valued data sets was previously developed (Kraskov et al. 2004). We present an accurate method for calculating MI between one discrete data set and one real-valued data set. For example, this calculator can quantify the correlation between base methylation (a discrete variable) and gene expression level (real-valued), or the effect of a clinical procedure (boolean; discrete) on patient survival time (real-valued). We use our